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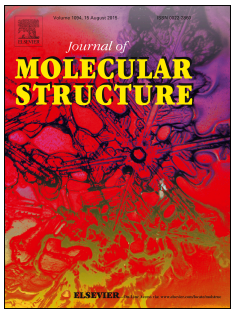

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ACCEPTED MANUSCRIPT

Crystallographic, thermal and spectroscopic characterization of the anhydrous thiourea−barbituric acid and thiourea−2-thiobarbituric acid co-crystals

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Abstract

Thiourea (Tu) crystallizes with barbituric acid (H_2ba) and 2-thiobarbituric (H_2tba) in the aqueous solution to yield co-crystals H_2ba·Tu (**1**) and H_2tba·Tu (**2**). Powder of **1** was also obtained from individual compounds *via* kneading with H_2O. The structure of compounds was solved by the X-ray single crystal diffraction technique. In **1-2,** N—H···O, N—H···S, C—H···S and C—H···O hydrogen bonds form the different 3D nets. In structure **1**, centrosymmetric dimers of H_2ba and Tu molecules are formed by two N—H···O and N—H···S hydrogen bonds, respectively. These dimers alternate in one-dimensional tapes. In compound **2**, the same molecules are not bound by hydrogen bonds. Here, infinite chains are formed consisting of alternating molecules of H_2tba and Tu. In these chains, each of the molecules is connected to the other by two N—H···S hydrogen bonds. The compounds have been characterized by powder XRD, TG-DSC, and FT-IR.

Keywords: barbituric acid; 2-thiobarbituric acid; thiourea; X-ray diffraction; infrared spectroscopy

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